

3,3,3-Trifluoro-2,2-bis(trifluoromethyl)propanoic acid
917951-63-4 | DTXSID00633413

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 16.7 °C

Global applicability domain: Inside

Local applicability domain index: 3.70e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

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Heptafluorobutyric acid

Measured: -17.5

Predicted: -14.1

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Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-
dodecafluoro-

Measured: 34.0

Predicted: 32.9

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1,1,1,3,3,3-Hexafluoro-2-
propanol

Measured: -4.00

Predicted: -8.02

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PFOA

Measured: 55.0

Predicted: 53.2

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1-Nonanol,
2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-
hexadecafluoro-

Measured: 56.0

Predicted: 54.2